# 10/554,061

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ring bonds :
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exact bonds :
5-7 7-10
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isolated ring systems :
containing 1 :
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS
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1.3
         21 L2
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chain nodes :
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Page 1 of 13

13 14

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ring nodes :
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chain bonds :
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ring bonds :
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exact bonds :
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normalized bonds :
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isolated ring systems :
containing 1 : 7 :
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11:Atom 12:Atom 13:CLASS 14:CLASS
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=> s 13
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          21 L2
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=> s 16
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=> s 18 and pd <april 2003
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           11 L8 AND PD <APRIL 2003
=> s 111 and 112
L13
           0 L11 AND L12
=> dis 112 1-11 bib abs hitstr
L12 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:888735 CAPLUS Full-text
DM
    137:369971
    Preparation of substituted 4H-chromenes and analogs as activators of
    caspases and inducers of apoptosis and their uses against cancer and other
    disorders
```

Cai, Sui Xiong; Zhang, Hong; Jiang, Songchun; Storer, Richard

IN

Cytovia, Inc., USA PCT Int. Appl., 139 pp. CODEN: PIXXD2 Patent T.A English FAN.CNT 2 KIND DATE APPLICATION NO. DATE PATENT NO. \_\_\_\_\_ A1 20021121 WO 2002-US15399 ΡI WO 2002092594 20020516 <--W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG CA 2447010 A1 20021121 CA 2002-2447010 20020516 <--AU 2002314781 A1 20021125 AU 2002-314781 20020516 <--US 20030065018 20030403 US 2002-146138 A1 20020516 US 7053117 B2 20060530 EP 1392683 A1 20040303 EP 2002-741704 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR A CN 1516700 20040728 CN 2002-812067 20020516 JP 2004530692 т JP 2002-589478 20020516 20041007 US 20060035925 A1 20060216 US 2005-150586 20050613 PRAI US 2001-290997P P 20010516 US 1999-163584P P 19991105 US 2000-185211P P 20000224 A2 20001106 US 2000-705840 US 2002-146138 A1 20020516 WO 2002-US15399 W 20020516 MARPAT 137:369971 os

GI

PA

AB The present invention is directed to substituted 4H-chromenes and analogs thereof (shown as I; e.g. 2-amino-3-cyano-7-hydroxy-4-(3-bromo-4,5dimethoxyphenyl)-4H-chromene). It also relates to the discovery that I are activators of caspases and inducers of apoptosis and, therefore, can be used to induce cell death in a variety of clin. conditions in which controlled growth and spread of abnormal cells occurs. In I: R1-R4 = H, halo, haloalkyl, aryl, fused aryl, carbocyclic, heterocyclic, heteroaryl, C1-10 alkyl, alkenyl, alkynyl, arylalkyl, arylalkenyl, arylalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl, aminoalkyl, carboxyalkyl, nitro, amino, cyano, acylamido,

hydroxy, thiol, acyloxy, azido, alkoxy, carboxy, methylenedioxy, carbonylamido or alkylthio; or R1 and R2, or R2 and R3, or R3 and R4, taken together with the atoms to which they are attached form an aryl, heteroaryl, partially saturated carbocyclic or partially saturated heterocyclic group, wherein said group is optionally substituted. R5 is H or C1-10 alkyl; A is optionally substituted and is aryl, heteroaryl, saturated carbocyclic, partially saturated carbocyclic, saturated heterocyclic, partially saturated heterocyclic or arylalkyl; Y is CN, COR7, CO2R7 or CONRxRy, wherein R7, Rx and Rv = H. C1-10 alkvl, haloalkvl, arvl, fused arvl, carbocyclic, heterocyclic, heteroarvl, alkenyl, alkynyl, arvlalkyl, arvlalkenyl, arvlalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl or aminoalkyl; or Rx and Ry are taken together with the N to which they are attached to form a heterocycle; and Z is NR8R9, NHCOR8, N(COR9)2, N(COR8)(COR9), N:CHOR8 or N:CHR8, wherein R8 and R9 = H, C1-4 alkyl or aryl, or R8 and R9 are combined together with the group attached to them to form a heterocycle. The EC50 values for >80 I against T-47D and ZR-75-1 human breast cancer cell lines are tabulated, e.g. 30 and 25 nM, resp., for 2-amino-3-cyano-4-(3-bromo-4,5-dimethoxyphenyl)-4H-indolo[7,6-b]pyran. Although the methods of preparation are not claimed, 81 example prepns, are included.

- IT 70416-53-4, 5-Formylnicotinonitrile
  - RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of substituted 4H-chromenes and analogs as activators of caspases and inducers of apoptosis and their uses against cancer and other disorders)
- RN 70416-53-4 CAPLUS
- CN 3-Pyridinecarbonitrile, 5-formyl- (CA INDEX NAME)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:220560 CAPLUS Full-text

DN 136:263098

TI Preparation of pyridinyl amides and imides for use as fungicides

IN Neubert, Timothy Donald; Piotrowski, David Walter; Walker, Michael Paul

PA E. I. Du Pont de Nemours & Co., USA

SO PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.	CNT	1																	
	PA:	TENT :	.OV			KIN	D	DATE			APPL	ICAT	I NOI	NO.		D	ATE		
							-									-			
PI	WO	2002	0225	83		A2		2002	0321		WO 2	001-	US28	971		2	00109	917 -	<
	WO	2002	0225	83		A3		2002	0718										
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	PH,	PL,	
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ΤJ,	TM,	TR,	TT,	TZ,	UA,	UG,	
			US,	UZ,	VN,	YU,	ZA,	ZW											
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	

			DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
			ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
	ΑU	20020	1123	33		A		2002	0326		AU 2	002-	1123	3		2	0010	917	<
	BR	20010	1412	22		A		2003	0701		BR 2	001-	1412	2		2	0010	917	
	EP	13226	14			A2		2003	0702		EP 2	001-	9792	48		2	0010	917	
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY,	AL,	TR							
	JP	20045	1862	29		T		2004	0624		JP 2	002-	5268	36		2	0010	917	
	CN	16885	46			A		2005	1026		CN 2	001-	8155	19		2	0010	917	
	TW	23882	3			В		2005	0901		IW 2	001-	9012	3006		2	0010	919	
	za	20030	0064	13		A		2004	0219		ZA 2	003-	643			2	0030	123	
	IN	2003M	N001	L79		A		2005	0211		IN 2	003-	MN17	9		2	0030	205	
	US	20040	0440	40		A1		2004	0304		JS 2	003-	3802	43		2	0030	312	
	US	70747	42			B2		2006	0711										
	MX	2003P	A023	338		A		2003	0910		MX 2	003-	PA23	38		2	0030	317	
PRAI	US	2000-	2333	374P				2000	0918										
	US	2001-	2771	199P		P		2001	0320										
	WO	2001-	US28	3971		W		2001	0917										
OS	MAE	RPAT 1	36:2	26309	98														
CT																			

AB Title compds. [ACRRIR2YWB; A is a substituted pyridinyl ring; B is a substituted pyridinyl ring; W is C:L, SOn; L = O, S, CXR4; RI and R2 are each independently = H, Cl-C6 alkyl, C2-C6 alkeynl, C2-C6 alkynyl, C3-C6 cycloalkyl, each optionally substituted; Y = NR3; R3 = H, Cl-C6 alkyl, C2-C6 alkylaminocarbonyl, C3-C8 alkonyl, C2-C6 alkylaminocarbonyl, C3-C8 dislkylaminocarbonyl, R4 = C1-C6 alkyl, C2-C6 alkyn, C2-C6 alkyn, C2-C6 alkyn, C3-C8 cycloalkyl, each optionally substituted; X = O, S; n = 1, 2; provided that when W is CO and R1, R2 and R3 are H; then B is other than 4-trifluoromethyl-3-pyridinyl, 2-chloro-4-pyridinyl and 2,6-dihalo-4-pyridinyl, N-oxides and agriculturally suitable salts are prepared and disclosed which are useful as fungicides. Also disclosed are compns. containing the compds. I and a method for controlling plant diseases caused by fungal plant pathogens that involves applying an effective amount of a commound I.

IT 134031-24-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of pyridinyl amides and imides for use as fungicides)

RN 134031-24-6 CAPLUS

CN 3-Pyridinecarboxaldehyde, 2,4-dichloro- (CA INDEX NAME)

L12 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2001:85212 CAPLUS Full-text

DN 134:340420

II Unusual chemoselective addition of diisopropylzinc to 2,2"-bipyridine-5,5"dicarbonyl compounds in the 2-position and autoxidative reconversion with carbon-carbon bond cleavage

AU Tanji, Shigehisa; Shibata, Takanori; Sato, Itaru; Soai, Kenso

CS Department of Applied Chemistry, Faculty of Science, Science University of Tokyo, Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan

SO Journal of the Chemical Society, Perkin Transactions 1 (2001), (3), 217-218

CODEN: JCSPCE; ISSN: 1472-7781

PB Royal Society of Chemistry

DT Journal LA English

A English

OS CASREACT 134:340420 GI

 $\mathbb{R} \longrightarrow \mathbb{R}^1$ 

II

- AB Unusual chemoselective addition of diisopropylzinc to the 2-position of bipyridinedicarbonyl compds. I (R, Rl = CHO, CHO; COZMe, COZMe, Ac, COXMe2, COXMe2, COXMe2, H, CHO, H, COZMe, H, Ac; H, COXMe2) gave the adducts II with a quaternary carbon. Autoxidn. of II reconverts them into the initial compds. I with carbon-carbon bond cleavage.
- IT 338463-50-6P

RN

RL: SPN (Synthetic preparation); PREP (Preparation) (chemoselective addition of diisopropylzinc to bipyridinedicarbonyl compds. and autoxidn./carbon-carbon bond cleavage of dihydropyridylisopropylpyridines)

338463-50-6 CAPLUS

CN [2,2'-Bipyridine]-5-carboxaldehyde, 5'-(1-hydroxy-2-methylpropyl)- (CA INDEX NAME)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L12 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1999:723594 CAPLUS Full-text
- DN 132:58720
- TI Potent, Orally Active GPIIb/IIIa Antagonists Containing a Nipecotic Acid Subunit, Structure-Activity Studies Leading to the Discovery of RMJ-53308
- AU Hoekstra, William J.; Maryanoff, Bruce E.; Damiano, Bruce P.; Andrade-Gordon, Patricia; Cohen, Judith H.; Costanzo, Michael J.; Haertlein, Barbara J.; Hecker, Leonard R.; Hulshizer, Becky L.; Kauffman, Jack A.; Keane, Patricia; McComsey, David F.; Mitchell, John A.; Scott,
- Lorraine; Shah, Rekha D.; Yabut, Stephen C.

  Drug Discovery and New Product Research, The R. W. Johnson Pharmaceutical
  Research Institute. Spring House, PA. 19477, USA
- SO Journal of Medicinal Chemistry (1999), 42(25), 5254-5265 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
  - LA English
  - OS CASREACT 132:58720
  - AB Although i.v. administered antiplatelet fibringgen receptor (GPIIb/IIIa) antagonists have become established in the acute-care clin. setting for the prevention of thrombosis, orally administered drugs for chronic use are still under development. Herein, the authors present details from the authors exploration of structure-activity surrounding the prototype fibrinogen receptor antagonist RWJ-50042, which was derived from a unique approach involving the y-chain of fibrinogen (Hoekstra et al. J. Med. Chemical 1995, 38, 1582). The authors analog studies culminated in the discovery of RWJ-53308 (I), a potent, orally active GPIIb/IIIa antagonist. To progress from RWJ-50042 to a suitable candidate for clin. development, the authors conducted a series of optimization cycles that employed solid-phase parallel synthesis for the rapid, efficient preparation of nearly 250 analogs, which were assayed for fibrinogen receptor affinity and inhibition of platelet aggregation induced by four different activators. This strategy produced several promising analogs for advanced study, including the 3-(3,4-methylenedioxybenzene)- $\beta$ amino acid analog (significant improved in vivo potency) and the 3-(3pyridyl)-β-amino acid I (significantly improved potency, oral absorption, and duration of action). In dogs, I displayed significant ex vivo antiplatelet activity on oral administration at 1.0 mg/kg, 16% systemic oral bioavailability, minimal metabolic transformation, and an excellent safety profile. Addnl., I was efficacious in three in vivo thrombosis models: canine arteriovenous (AV) shunt (0.01-0.1 mg/kg, iv), guinea pig photoactivationinduced injury (0.3-3 mg/kg, iv), and guinea pig ferric chloride-induced injury (0.3-1 mg/kg, iv). On the basis of its noteworthy preclin. data, I was selected for clin. evaluation.
  - IT 252989-56-3P
    - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
      - (potent, orally active GPIIb/IIIa antagonists containing a nipecotic acid subunit and structure-activity studies leading to discovery of RWJ-53308 as antiplatelet agent for treatment of thrombosis)
- RN 252989-56-3 CAPLUS
- CN 3-Pyridinecarboxaldehyde, 5-(2-phenylethynyl)- (CA INDEX NAME)



#### RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

1997:609624 CAPLUS Full-text

DN 127:262666

OREF 127:51301a,51304a

Naphthyridine derivatives, their methods of preparation and pharmaceutical compositions containing them, useful especially as antiproliferative drugs IN Bru-Magniez, Nicole; Launay, Michele; Teulon, Jean-Marie

PA Laboratoires UPSA, Fr.

U.S., 11 pp., Cont.-in-part of U.S. 5,364,860.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2	
PATENT	NO.

E Pars.	CIVI	2																	
	PA:	TENT :	NO.			KIN	D									DF	ATE		
PI	US	5663	181			A		1997	0902		US 1	995-	5496	65		19	1951:	129	<
	FR	2706	898			A1		1994	1230		FR 1	993-	7746			19	930	525	<
	FR	2706	898			В1		1995	0908										
	US	5364	860			A		1994	1115		US 1	993-	9723	9		19	930	727	<
	WO	9500	513			A1		1995	0105		WO 1	994-	FR76	3		19	940	524	<
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																MN,			
																US,			
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									GA,										
	ΑU	9471	275			A		1995	0117		AU 1	994-	7127	5		19	940	524	<
	EP	7052	61			A1		1996	0410		EP 1	994-	9205	07		19	940	524	<
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	LI,	LU,	MC,	NL,	PT,	SE
	JP	0851	1793			T		1996	1210		JP 1	994-	5025	24		19	9400	524	<
	FI	9504	982			A		1995	1227		FI 1:	995-	4982			19	9510	019	<
PRAI		1993						1993	0625										
	US	1993	-972	39		A2		1993	0727										
	WO	1994	-FR7	63		W		1994	0624										
OS MARPAT 127:262666																			
GI																			

Page 8 of 13

II

- The invention relates to title compds. I [X = H, halo; Y = O, S, NH; R, R1 =H, cyano, CO2R'; CONH2, CONH(CH2) nC6H4R'', NO2, pyridyl, halopyridyl, thiazolyl, alkylthiazolyl; or RR1 form indolin-2-one; R2 = alkyl, cycloalkyl, (CH2)mC6H3Z1Z2; m, n = 0-5; R' = H, alkyl; R'' = H, halo, alkyl; Z1, Z2 = H, alkyl, halo, CF3, OH, alkoxy, alkylthio, NO2, NH2, cyano] and their addition salts. The compds. are useful as drugs having antiproliferative properties, affording an effective treatment for diseases such as cancer, psoriasis, atherosclerosis, restenosis phenomena, or any other pathol. condition due to cell proliferation. For instance, condensation of 1-(3,5-dichlorophenyl)-1,2dihydro-2-oxo-1,8-naphthyridine- 3-carboxaldehyde (preparation given) with 4pyridylacetonitrile-HCl in EtOH in the presence of NaOEt gave 40% title compound II, a preferred compound In an assay for inhibition of PDGFstimulated proliferation of balb c 3T3 fibroblasts in culture, II had an IC50 of 0.2 µM. Preliminary toxicol. studies showed good tolerance in rats at up to 300 mg/kg orally or i.p. IT 195883-62-6P
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (intermediate; preparation of naphthyridine derivs. as antiproliferatives) RN 195883-62-6 CAPLUS
- CN 3-Pyridinecarboxaldehyde, 5-chloro-2-[(3,5-dichlorophenyl)amino]- (CA INDEX NAME)

- L12 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1991:449586 CAPLUS Full-text
- DN 115:49586
- OREF 115:8612h,8613a
- TI Lithiation of polychloropyrimidines and dichloropyridines
- AU Radinov, R.; Chanev, Kh.; Khaimova, M.
- CS Fac. Chem., Univ. Sofia, Sofia, 1126, Bulg.
- SO Journal of Organic Chemistry (1991), 56(15), 4793-6
- CODEN: JOCEAH; ISSN: 0022-3263
- DT Journal
- LA English
- OS CASREACT 115:49586
- AB Polychloropyrimidines and -pyridines bearing halogens at activated ring positions can be regioselectively metalated with (Me2CH)2NLi or Bull in THF at -80°. Lithiated heterocycles react with electrophiles to give adducts in high yield. The unusual C-4 selectivity of lithiation of 2,6-dichloropyridine with Buli was studied. Trapping of lithiated intermediates with PhCHO and
- subsequent oxidation afforded useful heterocyclic building blocks.
- IT 134031-24-6P
  - RL: SPN (Synthetic preparation); PREP (Preparation)
    (preparation of)
- RN 134031-24-6 CAPLUS
- CN 3-Pyridinecarboxaldehyde, 2,4-dichloro- (CA INDEX NAME)

L12 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1981:569014 CAPLUS Full-text

DN 95:169014

OREF 95:28249a,28252a

Pyridinyloxypropanolamines

Baldwin, John J.; Ponticello, Gerald S. IN

Merck and Co., Inc., USA

SO U.S., 14 pp. Cont.-in-part of U.S. Ser. No. 866,961, abandoned.

CODEN: USXXAM

DT Patent LA. English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
PI	US 4279913	A	19810721	US 1979-7092	19790129 <			
	JP 54106476	A	19790821	JP 1978-164500	19781229 <			
	DK 7900023	A	19790807	DK 1979-23	19790103 <			
	US 4294969	A	19811013	US 1980-167577	19800711 <			
	US 4393212	A	19830712	US 1981-263335	19810513 <			
PRA	I US 1978-866961	A2	19780104					
	US 1979-7092	A3	19790129					
OS	CASREACT 95:169014	1						

GI

- AB Pyridinyloxypropanolamines I (n = 1, 2; R = C3-4 branched alkyl; R1 = H, acyl) were prepared for use as  $\beta$ -sympatholytics and antihypertensives (no data). Thus, cyclopentylidenemalononitrile was treated with HC(OEt)3 and cyclized with HBr-HOAc to give 57% 2-bromo-3- cyanocyclopenta[c]pyridine which was treated with (S)-2-phenyl-3-tert- butyl-5-hydroxymethyloxazolidine to give 35% I (R = CMe3, R1 = H, n = 1).
- ΙT 70416-53-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 70416-53-4 CAPLUS RN

CN 3-Pyridinecarbonitrile, 5-formyl- (CA INDEX NAME)

L12 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN 1979:474426 CAPLUS Full-text AN DN 91:74426 OREF 91:12029a,12032a Functionalization of 5-methyl-2-halonicotinic acid derivatives AU Ponticello, Gerald S.; Baldwin, John J. CS Dep. Med. Chem., Merck Sharp and Dohme Res. Lab., West Point, PA, 19486, USA SO Journal of Organic Chemistry (1979), 44(15), 2702-4 CODEN: JOCEAH; ISSN: 0022-3263 DT Journal LA English AB Pyridines containing versatile functional groups in the 2, 3, and 5 positions were prepared via N-bromosuccinimide di- and tribrominations of the C-5 Me group of 2-halonicotinic acid derivs. Reductive dehalogenation of the 2-bromo substituent provides for a facile synthesis of unsym. pyridines in which the

oxidation state of the C-3 and C-5 groups can be effectively controlled.

- тт 70416-53-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- RN 70416-53-4 CAPLUS
- 3-Pyridinecarbonitrile, 5-formyl- (CA INDEX NAME) CN

- L12 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
- 1978:538018 CAPLUS Full-text AN
- DN 89:138018
- OREF 89:21249a,21252a
- Moessbauer spectra of bidentate and monodentate carbonyl-substituted pyridine complexes of iron(II) dichlorides
- Wei, Ho-Hsiang; Men, Lee-Chung AU
- CS Dep. Chem., Tamkang Coll. Art Sci., Tamsui, Taiwan
- Journal of Inorganic and Nuclear Chemistry (1978), 40(2), 221-4 SO
- CODEN: JINCAO; ISSN: 0022-1902 DT
- Journal
- LA English
- AB Thirteen complexes FeL2Cl2 (L = 2-, 3-, or 4-carbonyl-substituted pyridine) were prepared and characterized by Moessbauer and IR spectroscopy and magnetic moment measurements. FeL2Cl2 have distorted octahedral structures. The quadrupole splittings of the 2-substituted pyridine complexes are much larger than those of the 3- and 4-substituted pyridine complexes. The 2-substituted pyridines are bidentate whereas the 3- and 4-substituted pyridines are unidentate. The ground-state 3d orbital of the Fe in the complexes was shown to be dxv and the energy sepns, of the levels were estimated. The effect of the substituent on the isomer shift of the complexes is discussed.
- 65584-16-9P
- RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and Moessbauer spectrum of)
- RN 65584-16-9 CAPLUS
- CN Iron, dichlorobis(3-pyridinecarboxaldehyde-N1)-, (T-4)-, homopolymer (9CI)

(CA INDEX NAME)

CM 1

CRN 65584-15-8

CMF C12 H10 C12 Fe N2 O2

CCI CCS

L12 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1978:82940 CAPLUS Full-text

DN 88:82940

OREF 88:12977a,12980a

- TI Moessbauer spectra of bidentate and monodentate carbonyl-substituted pyridine complexes of iron(II) chlorides
- AU Wei, Ho-Hsiang; Men, Lee-Chung
- CS Dep. Chem., Tamkang Coll. Arts Sci., Tamsui, Taiwan
- SO Proceedings of the National Science Council [Taiwan], Part 1, Natural and Mathematical Sciences (1977), 10, 161-73 CODEN: PNSSDV. 15SN. 0378-2727
- DT Journal
- LA English
- AB Fei2Cl2, with pyridine derivs., RCSH4N(L; R = 2-, 3-, 4-MeCO, 2-, 3-, 4-PhCO, 2-, 4
- IT 65584-16-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and Moessbauer spectrum of)

RN 65584-16-9 CAPLUS

CN Iron, dichlorobis(3-pyridinecarboxaldehyde-N1)-, (T-4)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 65584-15-8

CMF C12 H10 C12 Fe N2 O2

CCI CCS

- L12 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1971:53445 CAPLUS Full-text
- DN 74:53445
- OREF 74:8605a,8608a
- TI Pyridines. VII. Hydration of diformylpyridines and their N-oxides
- AU Queguiner, Guy; Salaun-Bouix, Michele; Pastour, Paul
- CS Lab. Chim. Org., Inst. Nat. Super. Chim. Ind. Rouen, Mont-Saint-Aignan, Fr.
- SO Bulletin de la Societe Chimique de France (1970), (10), 3690-7
- CODEN: BSCFAS; ISSN: 0037-8968
- DT Journal
- LA French
- AB The hydration of diformylpyridines and their N-oxides by D2O was studied by NMR spectrometry. Thus, the 3,5-, 2,4-, 2,5-, and 2,6-diformylpyridine N-oxides gave 40, 50, 65, and 75% dihydrate. The 2,3- and 3,4-diformylpyridine N-oxides were completely hydrated as cyclic hydrates.
- IT 31198-35-3P
  - RL: SPN (Synthetic preparation); PREP (Preparation)
    (preparation of)
- RN 31198-35-3 CAPLUS
- CN Nicotinaldehyde, 5-(dihydroxymethyl)- (8CI) (CA INDEX NAME)

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